The Weyl Series and the Trace formula: Can we add them?

R. K. Bhaduri, N. D. Whelan

Department of Physics and Astronomy, McMaster University, Hamilton, Ontario L8S 4M1, Canada

M. Brack[1], H. G. Miller[2], M. V. N. Murthy[3]

[1]*Institute of Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany*
[2]*Department of Physics, University of Pretoria, Pretoria 0002, South Africa*
[2]*Institute of Mathematical Sciences, Chennai 600113, India*

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Periodic orbit expressions for the density of states lead to spurious results when directly used to calculate quantities of thermodynamic interest. This is because the trace formula is usually valid only for large energies while the calculations make use of it at all energies. We present a prescription for circumventing this problem by isolating contributions which arise from the inaccurate low-energy behavior, and are spurious, from other subdominant contributions which are physical and are not contained in the Weyl series. The method is tested by analyzing the fermionic grand partition function for a disk billiard and may readily be extended to other dynamical systems.

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In many-body systems such as atomic nuclei, metal clusters, quantum dots and traps with a dilute gas of bosons, much of the physics may be unraveled from the quantum description of the single particle motion in an appropriate mean field. Much effort has gone into developing intuitive, semiclassical descriptions of single-particle quantum dynamics [1–5]. One ubiquitous concept is the division of the density of states into two components, each with a distinct semiclassical interpretation. The first varies smoothly with energy and other parameters and is related to the geometrical properties of the classical phase space; for billiard systems this is the well-known Weyl series. The second component is an oscillatory function and is related to the dynamics of the classical system through various trace formulas. Balian and Bloch [3] showed that the decomposition can be made exact at the price of expressing the result in terms of certain integral representations. In practice, this is not very helpful and one is led to the expedient of expanding these out as asymptotic series. This leads to the Weyl term plus an infinite sum over periodic orbits, each one of which has its own asymptotic expansion in powers of $\hbar$. (Explicit higher order terms in the trace formulas for more than one dimension have been worked out only in a few trial systems [5,6].) We will refer to the sum over the periodic orbits to leading order in $\hbar$ as the trace formula. In the resulting approximation, however, it is not immediately clear to what extent this leads to spurious results in integrated quantities derived from the trace formula. The focus of this paper is to investigate this question, given a representation of the density of states as an infinite asymptotic Weyl series plus the trace formula. Certainly, this is the form in which the semiclassical results are most commonly expressed and used [1,5]. We would like to know to what extent we can meaningfully use this as it stands: for example in using it to calculate quantities of thermodynamic interest by integrating over it with various weight functions. The short answer is that we can not. The Weyl formula will typically have terms which cannot be integrated directly from zero energy. This problem is, however, easily circumvented by judicious integrations by parts [7]. A more serious problem, investigated here, is related to the fact that the trace formula is usually inaccurate at small energies and can lead to grossly incorrect results for the integrated quantities. We will show that this problem can be overcome by identifying a spurious component, which is due to the incorrect low-energy behavior. There is another component that is subdominant but contains the real, physical information about the periodic orbits.

In this paper we focus on the disk billiard, in part because its Weyl expansion is known to very high order [8] and also because of its physical importance, for example in quantum dots [9]. However, at the end we mention analogous results for a variety of systems in both two and three dimensions. For the disk, it is shown in [8] that the divergence of the higher-order terms in the Weyl series is controlled asymptotically by the shortest accessible periodic orbit through the phenomenon of resurgence [10,11]. The intricate link between the trace formula and the Weyl series has also been studied by Cartier and Voros [12,13]. Another interesting system to study in this regard is the harmonic oscillator [7] where there is an exact trace formula. Since it can be found by resummation of the Weyl series, we can work with either form. There are no spurious terms although there are still contributions from the periodic orbits which are exponentially small in temperature, as we will find for the disk.

We begin with the following decomposition of the quantum density of states: $\rho(E) = \sum_n \delta(E - E_n) \approx \overline{\rho}(E) + \delta\rho(E)$. The Weyl part $\overline{\rho}(E)$ is given in terms of reciprocal powers of E as well as delta functions and their derivatives. (The corresponding expression for the partition function is simpler and is presented below.)

The trace formula for the oscillating part $\delta\rho(E)$ (with $\hbar^2/2m = 1$ and disk radius $R = 1$) is given by [5,14]

$$\delta\rho(E) \approx \sum_{v=2}^{\infty} \sum_{w=1}^{[v/2]} \frac{A_{vw}}{E^{1/4}} \sin(\sqrt{E}L_{vw} + \theta_v), \qquad (1)$$

valid for $E \gg 1$. Each pair of integers (v, w) represents a one-parameter family of orbits, related by continuous rotations, where v is the number of vertices (i.e., reflections from the boundary of the disk) and w is the winding number. $L_{vw} = 2v\sin(\pi w/v)$ is the length of an orbit, $A_{vw} = f_{vw}L_{vw}^{3/2}/\sqrt{8\pi}v^2$ its amplitude and $\theta_v = (3\pi/4 - 3v\pi/2)$ its phase. The degeneracy factor f_{vw} is unity for $v = 2w$, otherwise it equals 2. We now consider using this expression to calculate physical observables of interest. As an example we consider the fermionic grand partition function [15] for non-interacting particles, from which all thermodynamic quantities can be derived:

$$\ln Z_G(\alpha, \beta) = \int_0^{\infty} \rho(E) \ln\left[1 + \exp(\alpha - \beta E)\right] dE. \quad (2)$$

Here β is the reciprocal temperature and $\alpha/\beta = \mu$ is the chemical potential. However the considerations of this paper will apply to any quantity expressible as an integral over the density of states, such as the total energy of a many-fermion system or the integrated density of states.

To proceed it is convenient to introduce the one-body partition function

$$Z(s) = \int_0^{\infty} \rho(E) \exp(-sE) \, dE. \qquad (3)$$

The parameter s can be thought of as an inverse temperature for the one-body problem. In what follows we will allow it to be complex, and for the present purpose it is just used as a mathematical variable. Noting that the *two-sided* Laplace transform of $\ln[1 + \exp(\alpha)]$ is $\pi/s\sin(\pi s)$ and using the convolution theorem [17] we can rewrite Eq. (2) in the form

$$\ln Z_G(\alpha, \beta) = \frac{1}{2\pi i} \int_C ds\, e^{\alpha s} \left\{ \frac{\pi}{s\sin(\pi s)} Z(\beta s) \right\}. \quad (4)$$

The contour C runs from $-i\infty$ to $i\infty$ with the real part of s between 0 and 1, although obviously this can be deformed within the rules of complex calculus. The study of the grand partition function has the nice feature of being directly related to physical observables. It has also the following mathematical advantage. It is well known that the trace formula for the single-particle density of states is generally divergent. However the finite temperature mitigates this. The number of orbits in the disk increases as a power law with orbit length while the temperature causes an exponential suppression with temperature. The net effect is a convergent sum.

Substituting $\overline{\rho}(E)$ into (3), one obtains

$$\overline{Z}(s) = \frac{c_0}{s} + \sum_{r=1}^{\infty} \frac{c_r}{\Gamma(r/2)} s^{r/2-1} \qquad (5)$$

with $c_0 = 1/4$, $c_1 = -\pi/4$, $c_2 = 1/6$, $c_3 = \pi/256$, etc. Berry and Howls [8] tabulate the coefficients up to c_{31}. This expression for $\overline{Z}$ may be substituted in Eq.(4) to obtain the Weyl series for the grand potential. We find

$$\overline{\ln Z_G}(\alpha, \beta) = \frac{c_0}{\beta} \int_0^{\infty} dE \ln(1 + e^{\alpha - E}) \qquad (6)$$

$$+ \sum_{n=1}^{N} \frac{c_{2n}}{\Gamma(n)} \beta^{n-1} \frac{d^{n-1}}{d\alpha^{n-1}} \ln(1 + e^{\alpha})$$

$$+ \sum_{n=0}^{N} \frac{c_{2n+1}}{\Gamma(n+1/2)} \beta^{n-1/2} \frac{d^n}{d\alpha^n} \int_0^{\infty} dE \frac{1}{\sqrt{\pi E}} \ln(1 + e^{\alpha - E}).$$

This series is asymptotic and diverges if taken to infinite order; it may therefore only be summed up to a maximum value N of the index n. This is shown in Fig. 1, where the difference

$$\Delta(\alpha, \beta) = \ln Z_G(\alpha, \beta) - \overline{\ln Z_G}(\alpha, \beta) \qquad (7)$$

between the quantum and the Weyl value is plotted versus N (circles) for selected fixed values of α and β. For $\mu = \alpha/\beta \gg 1$, Δ settles down to a plateau after a few terms of the series, giving the optimum result. The asymptotic nature of the series (6) is apparent for $\alpha/\beta = 1$ in the bottom of Fig. 1, where $|\Delta|$ is seen to increase rapidly with the inclusion of higher order terms. (The same happens for the other cases, but at higher values of N.) We see from this figure that the series yields a plateau at a nonzero value, indicating that (6) deviates significantly from the true quantum result. This is reminiscent of the phenomenon discussed by Balian *et al.* [16] where it is shown how the error in using a given asymptotic expansion can be dominated not by the least term in the expansion used but rather in neglecting some weaker subdominant saddle contribution. Clearly what is missing here is the contribution from the periodic orbits.

We proceed by substituting into (2) the oscillating density of states as given by (1). This gives a spurious result. For example, in the limit $\beta = 0$ we are left with simple Fresnel integrals. Upon doing the sum over orbits we get the finite contribution $(\ln 2 - \pi^2/24)\ln(1 + e^{\alpha})/4\sqrt{2}$. However, we know that in this limit the Weyl contribution is exact and clearly adding this amount would destroy the agreement. Therefore, we should not take the prescription of substituting the oscillating density of states into (2) too literally.

Rather, we proceed as before by first calculating the contribution to the one-body partition function. Changing variables to $k = \sqrt{E}$ we have the following integral to do for each orbit

$$\int_0^{\infty} dk \sqrt{k} \sin(kL + \theta) \exp(-sk^2), \qquad (8)$$

where we have temporarily suppressed the v and w indices. We decompose the sinusoid into two exponentials and then separately analyze the two integrals. There is an end-point contribution from the lower limit which can be determined from Watson's lemma [10]. There is also a saddle at either of $k = \pm iL/2s$ which may or may not contribute depending on the phase of s; there is a Stoke's phenomenon when $\Im s = 0$. The final result valid for $|s| \ll 1$ is [18]

$$\delta Z_{\mathrm{s}}(s) \approx -\sum_{\substack{\mathrm{v,w} \\ \mathrm{v\ even}}} f_{\mathrm{vw}} \frac{(-)^{\mathrm{v}/2}}{\sqrt{8}\mathrm{v}^2} \sum_{n=0}^{N_{\mathrm{s}}} \frac{(4n+1)!!}{2^{2n}n!} \left(\frac{s}{L_{\mathrm{vw}}^2}\right)^n, \quad (9)$$

$$\delta Z_{\mathrm{p}}(s) \approx \sum_{\mathrm{v,w}} \frac{f_{\mathrm{vw}}}{4\mathrm{v}^2} L_{\mathrm{vw}}^2 \frac{e^{-L_{\mathrm{vw}}^2/4s}}{s} e^{\pm i(\theta_{\mathrm{v}} - \pi/4)}, \quad (10)$$

where the upper and lower signs in the phase of (10) hold for $\Im s \gtrless 0$. When $\Im s = 0$, one should take the mean of the two expressions [10]. The sum over n in (9) is asymptotic and must be truncated at some maximum value N_{s} that depends on the orbit. The series (9) comes from the end-point analysis. When substituted into (4), its first term is the unwanted contribution at $\beta = 0$ mentioned earlier. In fact, the entire series is unwanted. It results in power series contributions to $\ln Z_G$, but we have already shown in Eq. (6) that its power series is correctly generated by the Weyl series alone. Therefore this entire series is spurious — hence the subscript s — and is neglected in what follows. This will be justified more rigorously below. The second contribution (10), by contrast, comes from the saddle-point analysis. We will see that it does contain the physical information about the contributions of the periodic orbits — hence the subscript p. It is interesting to note that (10) is exponentially subdominant compared to (9) and yet carries all the relevant information. Higher-order saddle-point corrections to (10) have been worked out [19], but there is no reason to include them here because they correspond to the missing higher-order corrections to the trace formula (1) which are unknown.

The origin of the spurious series (9) is the low-energy region, where the trace formula is inaccurate. Removing this spurious series could be thought of as subtracting from (1) a series of the form $\delta\rho_{\mathrm{s}}(E) = \sum_{n=0}^{N_{\mathrm{s}}} a_n \delta^{(n)}(E)$. Requiring that all moments of the corrected trace formula be zero fixes the coefficients a_n and leads to subtraction of (9) from $\delta Z(s)$. Another argument for ignoring $\delta Z_{\mathrm{s}}(s)$ is as follows. The derivation of (1) assumes energy is large. We are therefore free to replace this expression by any other which is asymptotically the same. However, the expansion (9) is not invariant under such a change (unlike (10)) and we therefore conclude that it cannot contain any meaningful information. It is even possible to find a version of $\delta\rho(E)$ whose spurious contribution is identically zero by inverse Laplace transforming the

physical expression (10). This gives Bessel functions [7] whose asymptotic expansions are precisely $\delta\rho(E)$. However for small energy they behave more smoothly and, most importantly, do not lead to spurious structure. We interpret the result as a regularised trace formula.

We now calculate the contribution of the periodic orbits to the fermionic grand partition function by substituting $\delta Z_{\mathrm{p}}(s)$ into (4) (while omitting δZ_{s}) and doing the contour integral numerically. We call the result $(\delta \ln Z_G)_{\mathrm{p}}$ and show it in Table 1 for a few cases together with $\Delta(\alpha, \beta)$. Clearly this analysis captures the part missing from the Weyl series. We stress that this would certainly not be the case had we included the spurious series. We also show this data in Figure 1 as the dashed horizontal line. For comparison we also show the result of substituting (1) directly into (2), doing the integrals numerically and subtracting off the spurious series found from substituting (9) into the relation (4). The results are shown as crosses where the horizontal axis represents N_{s} in (9). The asymptotic result is well captured by $(\delta \ln Z_G)_{\mathrm{p}}$.

Thus, the contribution of periodic orbits to the grand potential accounts for the difference between the quantum and the Weyl calculations in a consistent manner, but only after discarding the spurious contributions. It is interesting to note that the periodic orbits represent a much more important contribution to $\ln Z_G$ than to Z itself, for reasons we do not have space to discuss here [7]. The integral (4) has saddles at $s = \pm iL/2\sqrt{\alpha/\beta}$ and the resulting stationary phase analysis leads to a known form [20] valid in the limit of large α. However, by doing the integral exactly we can relax this constraint and therefore have a more general result. (Both approaches fail, however, when μ becomes much smaller than one.)

This sort of analysis can immediately be generalized to other classes of periodic orbits. For example, a typical billiard orbit contributes to trace formulas as $AE^{n/4}\sin(\sqrt{E}L + \sigma\pi/2 + n\pi/4)$. Examples are diffractive orbits in two dimensions, isolated orbits, the disk orbits considered here, diameter orbits in the sphere and polygonal orbits in the sphere for which $n = (-3, -2, -1, 0, 1)$ respectively. In its contribution to $Z(s)$, we can identify a component which comes from the end point and is spurious and another which comes from a saddle point and is physical. The latter is approximately

$$A\sqrt{\pi}\left(\frac{L}{2}\right)^{n/2+1} \frac{e^{-L^2/4s}}{s^{(n+3)/2}} e^{\pm i(\sigma+n)\pi/2}, \quad (11)$$

which agrees with (10) for the case $n = -1$ with $\sigma \equiv 2 - 3\mathrm{v}$ and substituting in the amplitudes from (1). This can also be extended to potential systems, scaling or otherwise, although the former is somewhat simpler.

In summary, a careful asymptotic analysis of integrals over approximate trace formulas reveals that the physically relevant contributions from the periodic orbits are

contained in exponentially subdominant terms, whereas the dominant terms that come from the inaccurate low-energy behavior of $\delta\rho(E)$ are spurious and must be discarded. Adding only the subdominant terms to the Weyl series gives good numerical agreement with quantum-mechanical results.

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α	β	$\ln Z_G$	Δ	$(\delta \ln Z_G)_{\mathrm{p}}$
10	1.0	4.2499	0.2880	0.2549
10	0.5	12.6489	0.2144	0.2100
10	0.1	97.0390	-0.0075	-0.0071
1	1.0	0.0083	0.0148	0.0152

TABLE I. The logarithm of the grand partition function, the difference from the Weyl approximation and the contribution from the periodic orbits (with the spurious part removed) for a selection of values of α and β.
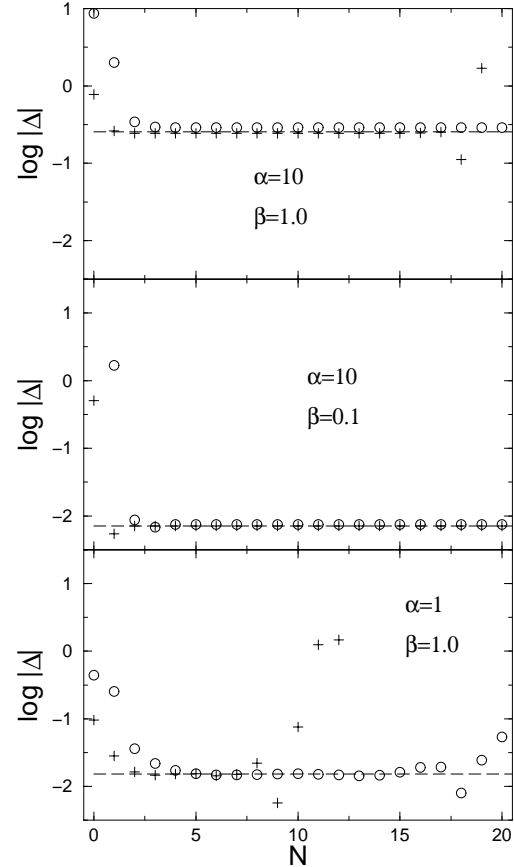

FIG. 1. The logarithm (base 10) of Δ versus the order in the asymptotic expansion (circles). The dashed line is the periodic orbit prediction $(\delta \ln Z_G)_{\mathrm{p}}$. The crosses result from directly using the expression (1) in the energy integral (2) and then explicitly subtracting off the spurious component versus N_{s} in (9).